Short-Range Spin Glasses: The Metastate Approach

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Abstract

We discuss the *metastate*, a probability measure on thermodynamic states, and its usefulness in addressing difficult questions pertaining to the statistical mechanics of systems with quenched disorder, in particular short-range spin glasses. The possible low-temperature structures of realistic (i.e., short-range) spin glass models are described, and a number of fundamental open questions are presented.

1 Introduction

The nature of the low-temperature spin glass phase in short-range models remains one of the central problems in the statistical mechanics of disordered systems [1, 2, 3, 4, 5, 6, 7]. While many of the basic questions remain unanswered, analytical and rigorous work over the past decade have greatly streamlined the number of possible scenarios for pure state structure and organization at low temperature, and have clarified the thermodynamic behavior of these systems.

The unifying concept behind this work is that of the *metastate*. It arose independently in two different constructions [8, 9], which were later shown to be equivalent [10]. The metastate is a probability measure on the space of all thermodynamic states. Its usefulness arises in situations where multiple "competing" pure states may be present. In such situations it may be difficult to construct individual states in a measurable and canonical way; the metastate avoids this difficulty by focusing instead on statistical properties of the states.

An important aspect of the metastate approach is that it relates, by its very construction [9], the observed behavior of a system in large but finite volumes with its thermodynamic properties. It therefore serves as a (possibly indispensable) tool for analyzing and understanding both the infinite-volume and finite-volume properties of a system, particularly in cases where a straightforward interpolation between the two may be incorrect, or their relation otherwise difficult to analyze.

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We will focus on the Edwards-Anderson (EA) Ising spin glass model [11], although most of our discussion is relevant to a much larger class of realistic models. The EA model is described by the Hamiltonian

$$\mathcal{H}_{\mathcal{J}} = -\sum_{\langle x,y \rangle} J_{xy}\sigma_x\sigma_y \quad , \tag{1}$$

where $\mathcal{J}$ denotes a particular realization of all of the couplings J_{xy} and the brackets indicate that the sum is over nearest-neighbor pairs only, with $x, y \in \mathbf{Z}^d$. We will take Ising spins, $\sigma_x = \pm 1$; although this will affect the details of our discussion, it is unimportant for our main conclusions. The couplings J_{xy} are quenched, independent, identically distributed random variables whose common distribution μ is symmetric about zero.

2 States and Metastates

We are interested in both finite-volume and infinite-volume Gibbs states. For the cube of length scale L, $\Lambda_L = \{-L, -L+1, \cdots, L\}^d$, we define $\mathcal{H}_{\mathcal{J},L}$ to be the restriction of the EA Hamiltonian to Λ_L with a specified boundary condition (b.c.) such as free or fixed or periodic. Then the finite-volume Gibbs distribution $\rho_{\mathcal{J}}^{(L)} = \rho_{\mathcal{J},\beta}^{(L)}$ on Λ_L (at inverse temperature $\beta = 1/T$) is:

$$\rho_{\mathcal{J},\beta}^{(L)}(\sigma) = Z_L^{-1} \exp\{-\beta\mathcal{H}_{\mathcal{J},L}(\sigma)\} \quad , \tag{2}$$

where the partition function $Z_L(\beta)$ is such that the sum of $\rho_{\mathcal{J},\beta}^{(L)}$ over all σ yields one. (In this and all succeeding definitions, the dependence on spatial dimension d will be suppressed.)

Thermodynamic states are described by *infinite*-volume Gibbs measures. At fixed inverse temperature β and coupling realization $\mathcal{J}$, a thermodynamic state $\rho_{\mathcal{J},\beta}$ is the limit, as $L \to \infty$, of some sequence of such finite-volume measures (each with a specified b.c., which may remain the same or may change with L). A thermodynamic state $\rho_{\mathcal{J},\beta}$ can also be characterized intrinsically through the Dobrushin-Lanford-Ruelle (DLR) equations [12]: for any Λ_L, the conditional distribution of $\rho_{\mathcal{J},\beta}$ (conditioned on the sigma-field generated by $\{\sigma_x : x \in \mathbf{Z}^d \backslash \Lambda_L\}$ is $\rho_{\mathcal{J},\beta}^{(L),\overline{\sigma}}$, where $\overline{\sigma}$ is given by the conditioned values of σ_x for x on the boundary of Λ_L.

Consider now the set $\mathcal{G} = \mathcal{G}(\mathcal{J}, \beta)$ of all thermodynamic states at a fixed $(\mathcal{J}, \beta)$. The set of extremal, or pure, Gibbs states is defined by

$$\mathrm{ex}\ \mathcal{G} = \mathcal{G} \setminus \{a\rho_1 + (1-a)\rho_2 :\ a \in (0,1);\ \rho_1, \rho_2 \in \mathcal{G};\ \rho_1 \neq \rho_2\}\,, \tag{3}$$

and the number of pure states $\mathcal{N}(\mathcal{J}, \beta)$ at $(\mathcal{J}, \beta)$ is the cardinality $|\mathrm{ex}\ \mathcal{G}|$ of ex $\mathcal{G}$. It is not hard to show that, in any d and for a.e. $\mathcal{J}$, the following two statements are true: 1) $\mathcal{N} = 1$ at sufficiently low $\beta > 0$; 2) at any fixed β, $\mathcal{N}$ is constant a.s. with respect to

the $\mathcal{J}$'s. (The last follows from the measurability and translation-invariance of $\mathcal{N}$, and the translation-ergodicity of the disorder distribution of $\mathcal{J}$.)

A pure state ρ_α (where α is a pure state index) can also be intrinsically characterized by a *clustering property*; for two-point correlation functions this reads

$$\langle \sigma_x \sigma_y \rangle_{\rho_\alpha} - \langle \sigma_x \rangle_{\rho_\alpha} \langle \sigma_y \rangle_{\rho_\alpha} \to 0 \tag{4}$$

as $|x-y| \to \infty$. A simple observation [13] with important consequences for spin glasses, is that if many pure states exist, a sequence of $\rho_{\mathcal{J},\beta}^{(L)}$'s, with b.c.'s and L's chosen independently of $\mathcal{J}$, will generally not have a (single) limit. We call this phenomenon *chaotic size dependence* (CSD).

We will be interested in the properties of ex $\mathcal{G}$ at low temperature. If the spin-flip symmetry present in the EA Hamiltonian Eq. (1) is spontaneously broken above some dimension d_0 and below some temperature $T_c(d)$, there will be at least a *pair* of pure states, such that their even-spin correlations are identical, and their odd-spin correlations have the opposite sign. Assuming that such broken spin-flip symmetry indeed exists for $d > d_0$ and $T < T_c(d)$, the question of whether there exists *more than one* such pair (of spin-flip related extremal infinite-volume Gibbs distributions) is a central unresolved issue for the EA and related models. If many such pairs should exist, we can ask about the structure of their relations to one another, and how this structure would manifest itself in large but finite volumes.

To do this we use an approach, introduced in Ref. [9], to studying inhomogeneous and other systems with many competing pure states. This approach, based on an analogy to chaotic dynamical systems, requires the construction of a new thermodynamic quantity which we call the *metastate,* which is a probability measure $\kappa_\mathcal{J}$ on the thermodynamic states. The metastate allows an understanding of CSD by analyzing the way in which $\rho_{\mathcal{J},\beta}^{(L)}$ "samples" from its various possible limits as $L \to \infty$.

The analogy with chaotic dynamical systems can be understood as follows. In dynamical systems, the chaotic motion along a deterministic orbit is analyzed in terms of some appropriately selected probability measure, invariant under the dynamics. Time along the orbit is replaced, in our context, by L and the phase space of the dynamical system is replaced by the space of Gibbs states.

In [9], we considered (as always, at fixed β, which will hereafter be suppressed for ease of notation) a 'microcanonical ensemble' κ_N in which each of the finite-volume Gibbs states $\rho_\mathcal{J}^{(L_1)}, \rho_\mathcal{J}^{(L_2)}, \ldots, \rho_\mathcal{J}^{(L_N)}$ has weight N^{-1}. The ensemble κ_N converges to a metastate $\kappa_\mathcal{J}$ as $N \to \infty$, in the following sense: for every (nice) function g on states (e.g., a function of finitely many correlations),

$$\lim_{N\to\infty} N^{-1} \sum_{\ell=1}^{N} g(\rho^{(L_\ell)}) = \int g(\Gamma)\, d\kappa_\mathcal{J}(\Gamma) \quad . \tag{5}$$

The information contained in $\kappa_\mathcal{J}$ effectively specifies the fraction of cube sizes L_ℓ which the system spends in different (possibly mixed) thermodynamic states Γ as $\ell \to \infty$.

A different, but in the end equivalent approach, based on $\mathcal{J}$-randomness, is due to Aizenman and Wehr [8]. Here one considers the random pair $(\mathcal{J}, \rho_{\mathcal{J}}^{(L)})$, defined on the underlying probability space of $\mathcal{J}$, and takes the limit $\kappa^\dagger$ (with conditional distribution $\kappa_{\mathcal{J}}^\dagger$, given $\mathcal{J}$), via finite dimensional distributions along some subsequence. We omit details here, and refer the reader to [8, 10]. We note, though, the important result that a *deterministic* subsequence of volumes can be found on which both (5) is valid and $(\mathcal{J}, \rho_{\mathcal{J}}^{(L)})$ converges, with $\kappa_{\mathcal{J}}^\dagger = \kappa_{\mathcal{J}}$ [10].

In what follows we use the term "metastate" as shorthand for the $\kappa_{\mathcal{J}}$ constructed using periodic b.c.'s on a sequence of volumes chosen independently of the couplings, and along which $\kappa_{\mathcal{J}} = \kappa_{\mathcal{J}}^\dagger$. We choose periodic b.c.'s for specificity; the results and claims discussed are expected to be independent of the boundary conditions used, as long as they are chosen independently of the couplings.

3 Low Temperature Structure of the EA Model

There have been several scenarios proposed for the spin glass phase of the Edwards-Anderson model at sufficiently low temperature and high dimension. These remain speculative, because it has not even been proved that a phase transition from the high-temperature phase exists at positive temperature in *any* finite dimension.

We noted earlier that, at sufficiently high temperature in any dimension (and at all nonzero temperatures in one and presumably two dimensions, though the latter assertion has not been proved), there is a unique Gibbs state. It is conceivable that this remains the case in all dimensions and at all nonzero temperatures, in which case the metastate $\kappa_{\mathcal{J}}$ is, for a.e. $\mathcal{J}$, supported on a single, pure Gibbs state $\rho_{\mathcal{J}}$. (It is important to note, however, that in principle such a trivial metastate could occur even if $\mathcal{N} > 1$; indeed, just such a situation of "weak uniqueness" [14, 15] happens in very long range spin glasses at high temperature [16, 17].)

A phase transition has been proved to exist [18] in the Sherrington-Kirkpatrick (SK) model [19], which is the infinite-range version of the EA model. Numerical [1, 20, 21, 22] and some analytical [23, 24] work has led to a general consensus that above some dimension (typically around three or four) there does exist a positive temperature phase transition below which spin-flip symmetry is broken, i.e., in which pure states come in pairs, as discussed below Eq. (4). Because much of the literature has focused on this possibility, we assume it in what follows, and will see that the metastate approach is highly useful in restricting the scenarios that can occur.

The simplest such scenario is a two-state picture in which, below the transition temperature T_c, there exists a single pair of global flip-related pure states $\rho_{\mathcal{J}}^\alpha$ and $\rho_{\mathcal{J}}^{-\alpha}$. In this case there is no CSD for periodic b.c.'s and the metastate can be written

$$\kappa_{\mathcal{J}} = \delta_{\frac{1}{2}\rho_{\mathcal{J}}^\alpha + \frac{1}{2}\rho_{\mathcal{J}}^{-\alpha}} \, . \tag{6}$$

That is, the metastate is supported on a single (mixed) thermodynamic state.

The two-state scenario that has received the most attention in the literature is the *droplet/scaling* picture [25, 26, 27]. In this picture a low-energy excitation above the ground state in Λ_L is a droplet whose surface area scales as l^{d_s}, with $l \sim O(L)$ and $d_s < d$, and whose surface energy scales as l^θ, with $\theta > 0$ (in dimensions where $T_c > 0$). More recently, an alternative picture has arisen [28, 29] in which the low-energy excitations differ from those of droplet/scaling in that their energies scale as $l^{\theta'}$, with $\theta' = 0$.

The low-temperature picture that has perhaps generated the most attention in the literature is the replica symmetry breaking (RSB) scenario [1, 6, 30, 31, 32, 33, 34, 35], which assumes a rather complicated pure state structure, inspired by Parisi's solution of the SK model [3, 36, 37, 38]. This is a many-state picture ($\mathcal{N} = \infty$ for a.e. $\mathcal{J}$) in which the ordering is described in terms of the *overlaps* between states. There has been some ambiguity in how to describe such a picture for short-range models; we start with the prevailing, or standard, view. Consider any reasonably constructed thermodynamic state $\rho_{\mathcal{J}}$ (see [10] for more details) — e.g, the *average* over the metastate $\kappa_{\mathcal{J}}$

$$\rho_{\mathcal{J}} = \int \Gamma \, d\kappa_{\mathcal{J}}(\Gamma) \quad . \tag{7}$$

Now choose σ and σ' from the product distribution $\rho_{\mathcal{J}}(\sigma)\rho_{\mathcal{J}}(\sigma')$. The overlap Q is defined as

$$Q = \lim_{L\to\infty} |\Lambda_L|^{-1} \sum_{x\in\Lambda_L} \sigma_x \sigma'_x \, , \tag{8}$$

and $P_{\mathcal{J}}(q)$ is defined to be its probability distribution.

In the standard RSB picture $\rho_{\mathcal{J}}$ is a mixture of infinitely many pure states, each with a specific $\mathcal{J}$-dependent weight W:

$$\rho_{\mathcal{J}}(\sigma) = \sum_\alpha W^\alpha_{\mathcal{J}} \rho^\alpha_{\mathcal{J}}(\sigma) \ . \tag{9}$$

If σ is drawn from $\rho^\alpha_{\mathcal{J}}$ and σ' from $\rho^\beta_{\mathcal{J}}$, then the expression in Eq. (8) equals its thermal mean,

$$q^{\alpha\beta}_{\mathcal{J}} = \lim_{L\to\infty} |\Lambda_L|^{-1} \sum_{x\in\Lambda_L} \langle\sigma_x\rangle_\alpha \langle\sigma_x\rangle_\beta \quad , \tag{10}$$

and hence $P_{\mathcal{J}}$ is given by

$$P_{\mathcal{J}}(q) = \sum_{\alpha,\beta} W^\alpha_{\mathcal{J}} W^\beta_{\mathcal{J}} \delta(q - q^{\alpha\beta}_{\mathcal{J}}) \quad . \tag{11}$$

The *self-overlap*, or EA order parameter, is given by $q_{EA} = q^{\alpha\alpha}_{\mathcal{J}}$ and (at fixed T) is thought to be independent of both α and $\mathcal{J}$ (with probability one).

According to the standard RSB scenario, the $W^\alpha_{\mathcal{J}}$'s and $q^{\alpha\beta}_{\mathcal{J}}$'s are non-self-averaging (i.e., $\mathcal{J}$-dependent) quantities, except for $\alpha = \beta$ or its global flip, where $q^{\alpha\beta}_{\mathcal{J}} = \pm q_{EA}$. The average $P_s(q)$ of $P_{\mathcal{J}}(q)$ over the disorder distribution of $\mathcal{J}$ is predicted to be a mixture of two delta-function components at $\pm q_{EA}$ and a continuous part between them.

However, it was proved in [39] that this scenario cannot occur, because of the translation-invariance of $P_{\mathcal{J}}(q)$ and the translation-ergodicity of the disorder distribution. Neverthelesss, the metastate approach suggests an alternative, nonstandard, RSB scenario, which we now describe.

The idea behind the nonstandard RSB picture (referred to by us as the nonstandard SK picture in earlier papers) is to produce the finite-volume behavior of the SK model to the maximum extent possible. We therefore assume in this picture that in each Λ_L, the finite-volume Gibbs state $\rho_{\mathcal{J}}^{(L)}$ is well approximated deep in the interior by a mixed thermodynamic state $\Gamma^{(L)}$, decomposable into many pure states ρ_{α_L} (explicit dependence on $\mathcal{J}$ is suppressed for ease of notation). More precisely, each Γ in $\kappa_{\mathcal{J}}$ satisfies

$$\Gamma = \sum_{\alpha_\Gamma} W_\Gamma^{\alpha_\Gamma} \rho_{\alpha_\Gamma} \tag{12}$$

and is presumed to have a nontrivial overlap distribution for σ, σ' from $\Gamma(\sigma)\Gamma(\sigma')$:

$$P_\Gamma(q) = \sum_{\alpha_\Gamma, \beta_\Gamma} W_\Gamma^{\alpha_\Gamma} W_\Gamma^{\beta_\Gamma} \delta(q - q_{\alpha_\Gamma \beta_\Gamma}) \tag{13}$$

as did $\rho_{\mathcal{J}}$ in the standard RSB picture.

Because $\kappa_{\mathcal{J}}$, like its counterpart $\rho_{\mathcal{J}}$ in the standard SK picture, is translation-covariant, the resulting *ensemble* of overlap distributions P_Γ is independent of $\mathcal{J}$. Because of the CSD present in this scenario, the overlap distribution for $\rho_{\mathcal{J}}^{(L)}$ varies with L, no matter how large L becomes. So, instead of averaging the overlap distribution over $\mathcal{J}$, the averaging must now be done over the states Γ *within the metastate* $\kappa_{\mathcal{J}}$, all at fixed $\mathcal{J}$:

$$P_{ns}(q) = \int P_\Gamma(q) \kappa_{\mathcal{J}}(\Gamma) d\Gamma\,. \tag{14}$$

The $P_{ns}(q)$ is the same for a.e. $\mathcal{J}$, and has a form analogous to the $P_s(q)$ in the standard RSB picture.

However, the nonstandard RSB scenario seems rather unlikely to occur in any natural setting, because of the following result:

Theorem [40]. Consider two metastates constructed along (the same) deterministic sequence of Λ_L's, using two different sequences of flip-related, coupling-independent b.c.'s (such as periodic and antiperiodic). Then with probability one, these two metastates are the same.

The proof is given in [40], but the essential idea can be easily described here. As discussed in Sec. 2, $\kappa_{\mathcal{J}} = \kappa_{\mathcal{J}}^\dagger$; but $\kappa_{\mathcal{J}}^\dagger$ is constructed by a limit of finite dimensional distributions, which means averaging over other couplings including ones near the system boundary, and hence gives the same metastate for two flip-related boundary conditions.

This invariance with respect to different sequences of periodic and antiperiodic b.c.'s means essentially that the frequency of appearance of various thermodynamic states $\Gamma^{(L)}$ in finite volumes Λ_L is *independent* of the choice of boundary conditions. Moreover, this same invariance property holds among any two sequences of *fixed* boundary conditions

(and the fixed boundary condition of choice may even be allowed to vary arbitrarily along any single sequence of volumes)! It follows that, with respect to changes of boundary conditions, the metastate is extraordinarily robust.

This should rule out all but the simplest overlap structures, and in particular the nonstandard RSB and related pictures (for a full discussion, see [40]). It is therefore natural to ask whether the property of metastate invariance allows *any* many-state picture.

There is one such picture, which we have called *chaotic pairs*, and which is fully consistent with metastate invariance (our belief is that it is the *only* many-state picture that fits naturally and easily into results obtained about the metastate.)

Here the periodic b.c. metastate is supported on infinitely many pairs of pure states, but instead of Eq. (12) one has

$$\Gamma = (1/2)\rho_{\alpha_\Gamma} + (1/2)\rho_{-\alpha_\Gamma}\,, \tag{15}$$

with overlap

$$P_\Gamma = (1/2)\delta(q - q_{EA}) + (1/2)\delta(q + q_{EA})\,. \tag{16}$$

So there is CSD in the states but not in the overlaps, which have the same form as a two-state picture in every volume. The difference is that, while in the latter case, one has the *same* pair of states in every volume, in chaotic pairs the pure state pair varies chaotically as volume changes. If chaotic pairs is to be consistent with metastate invariance in a natural way, then the number of pure state pairs should be *uncountable*. This allows for a 'uniform' distribution (within the metastate) over all of the pure states, and invariance of the metastate with respect to boundary conditions could follow naturally.

4 Open Questions

We have discussed how the metastate approach to the EA spin glass has narrowed considerably the set of possible scenarios for low-temperature ordering in any finite dimension, should broken spin-flip symmetry occur. The remaining possibilities are either a two-state scenario, like droplet/scaling, or the chaotic pairs picture if there exist many pure states at some (β, d). Both have simple overlap structures. The metastate approach appears to rule out more complicated scenarios like RSB, in which the approximate pure state decomposition in a typical large, finite volume is a nontrivial mixture of many pure state pairs.

Of course, this doesn't answer the question of which, if either, of the remaining pictures actually does occur in real spin glasses. In this section we list a number of open questions relevant to the above discussion.

Open Question 1. Determine whether a phase transition occurs in any finite dimension greater than one. If it does, find the lower critical dimension.

Existence of a phase transition does not necessarily imply two or more pure states below T_c. It could happen, for example, that in some dimension there exists a single pure

state at all nonzero temperatures, with two-point spin correlations decaying exponentially above T_c and more slowly (e.g., as a power law) below T_c. This leads to:

Open Question 2. If there does exist a phase transition above some lower critical dimension, determine whether the low-temperature spin glass phase exhibits broken spin-flip symmetry.

If broken symmetry does occur in some dimension, then of course an obvious open question is to determine the number of pure state pairs, and hence the nature of ordering at low temperature. A (possibly) easier question (but still very difficult), and one which does not rely on knowing whether a phase transition occurs, is to determine the zero-temperature — i.e., ground state — properties of spin glasses as a function of dimensionality. A ground state is an infinite-volume spin configuration whose energy (governed by Eq. (1)) cannot be lowered by flipping any finite subset of spins. That is, all ground state spin configurations must satisfy the constraint

$$\sum_{\langle x,y\rangle\in\mathcal{C}} J_{xy}\sigma_x\sigma_y \geq 0 \tag{17}$$

along any closed loop $\mathcal{C}$ in the dual lattice.

Open Question 3. How many ground state pairs is the $T = 0$ periodic boundary condition metastate supported on, as a function of d?

The answer is known to be one for $1D$, and a partial result [41, 42] points towards the answer being one for $2D$ as well. There are no rigorous, or even heuristic (except based on underlying *ansätze*) arguments in higher dimension.

An interesting — but unrealistic — spin glass model in which the ground state structure can be exactly solved (although not yet completely rigorously) was proposed by the authors [43, 44] (see also [45]). This "highly disordered" spin glass is one in which the coupling magnitudes scale nonlinearly with the volume (and so are no longer distributed independently of the volume, although they remain independent and identically distributed for each volume). The model displays a *transition* in ground state multiplicity: below eight dimensions, it has only a single pair of ground states, while above eight it has uncountably many such pairs. The mechanism behind the transition arises from a mapping to invasion percolation and minimal spanning trees [46, 47, 48]: the number of ground state pairs can be shown to equal $2^{\mathcal{N}}$, where $\mathcal{N} = \mathcal{N}(d)$ is the number of distinct global components in the"minimal spanning forest." The zero-temperature free boundary condition metastate above eight dimensions is supported on a uniform distribution (in a natural sense) on uncountably many ground state pairs.

Interestingly, the high-dimensional ground state multiplicity in this model can be shown to be *unaffected* by the presence of frustration, although frustration still plays an interesting role: it leads to the appearance of chaotic size dependence when free conditions are used.

Returning to the more difficult problem of ground state multiplicity in the EA model, we note as a final remark that there could, in principle, exist ground state pairs that are not in the support of metastates generated through the use of coupling-independent

boundary conditions. If such states exist, they may be of some interest mathematically, but are not expected to play any significant physical role. A discussion of these putative "invisible states" is given in [7].

Open Question 4. If there exists broken spin-flip symmetry at a range of positive temperatures in some dimensions, then what is the number of pure state pairs as a function of (β, d)?

Again, the answer to this is not known above one dimension; indeed, the prerequisite existence of spontaneously broken spin flip symmetry has not been proved in any dimension. A speculative paper by the authors [49], using a variant of the highly disordered model, suggests that there is at most one pair of pure states in the EA model below eight dimensions; but no rigorous arguments are known at this time.

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